Equilibrium sampling of hard spheres up to the jamming density and beyond

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Collaborators:
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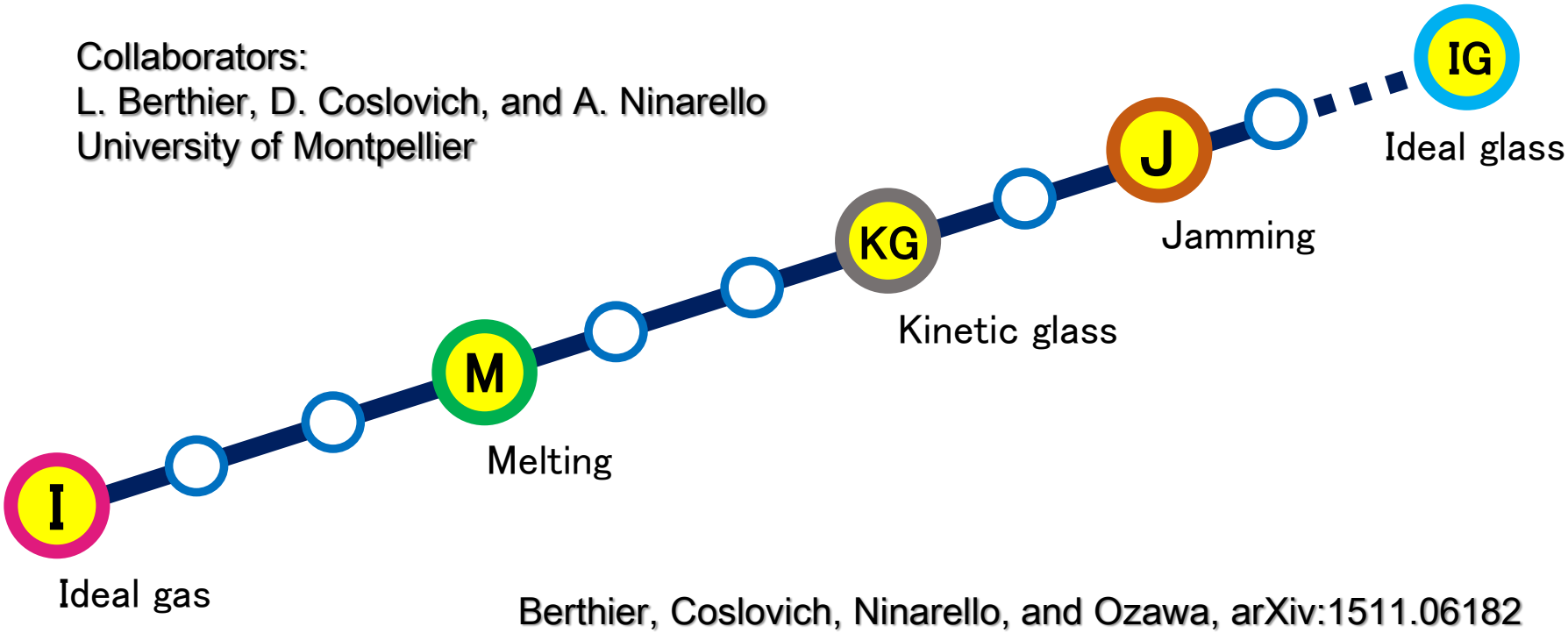
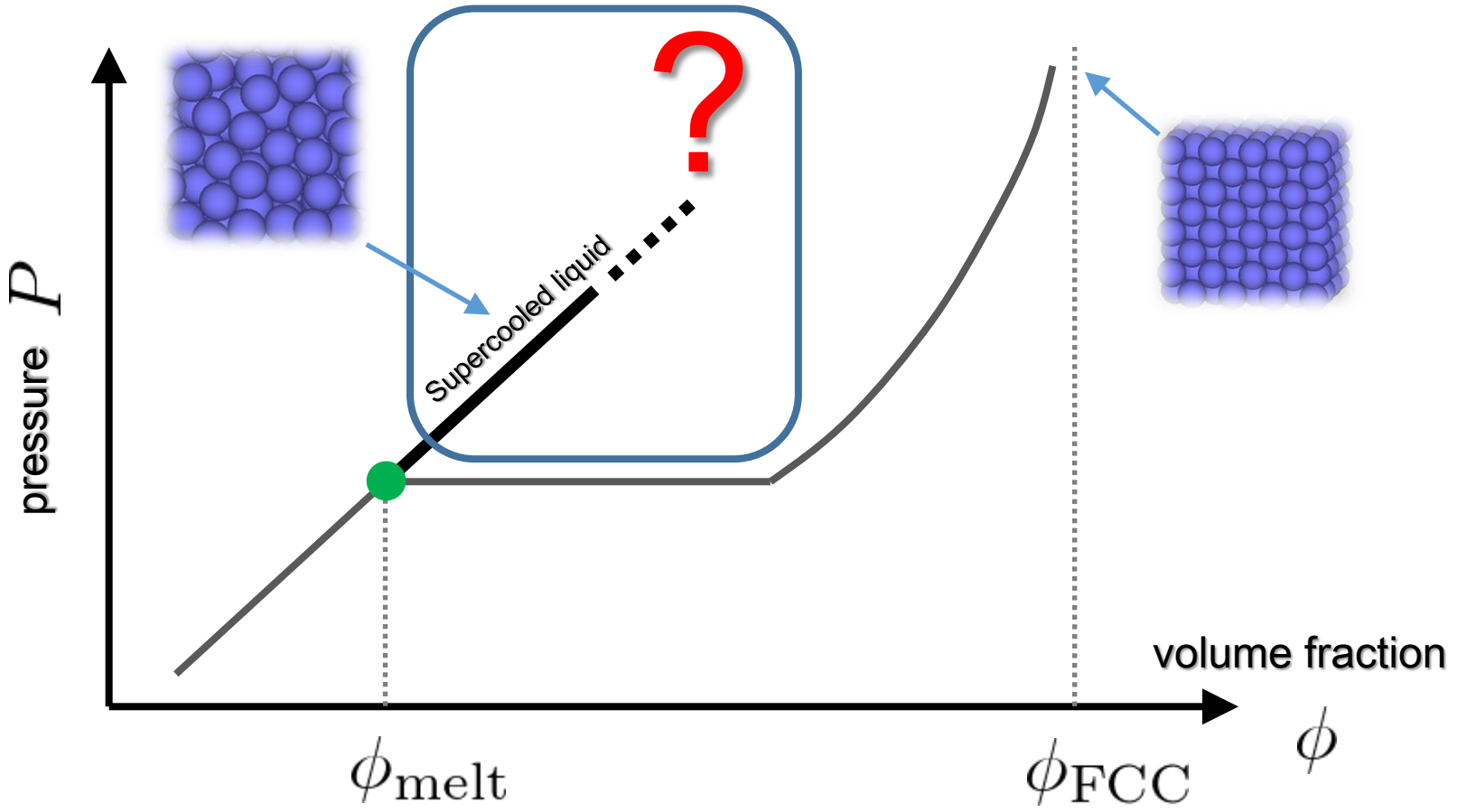
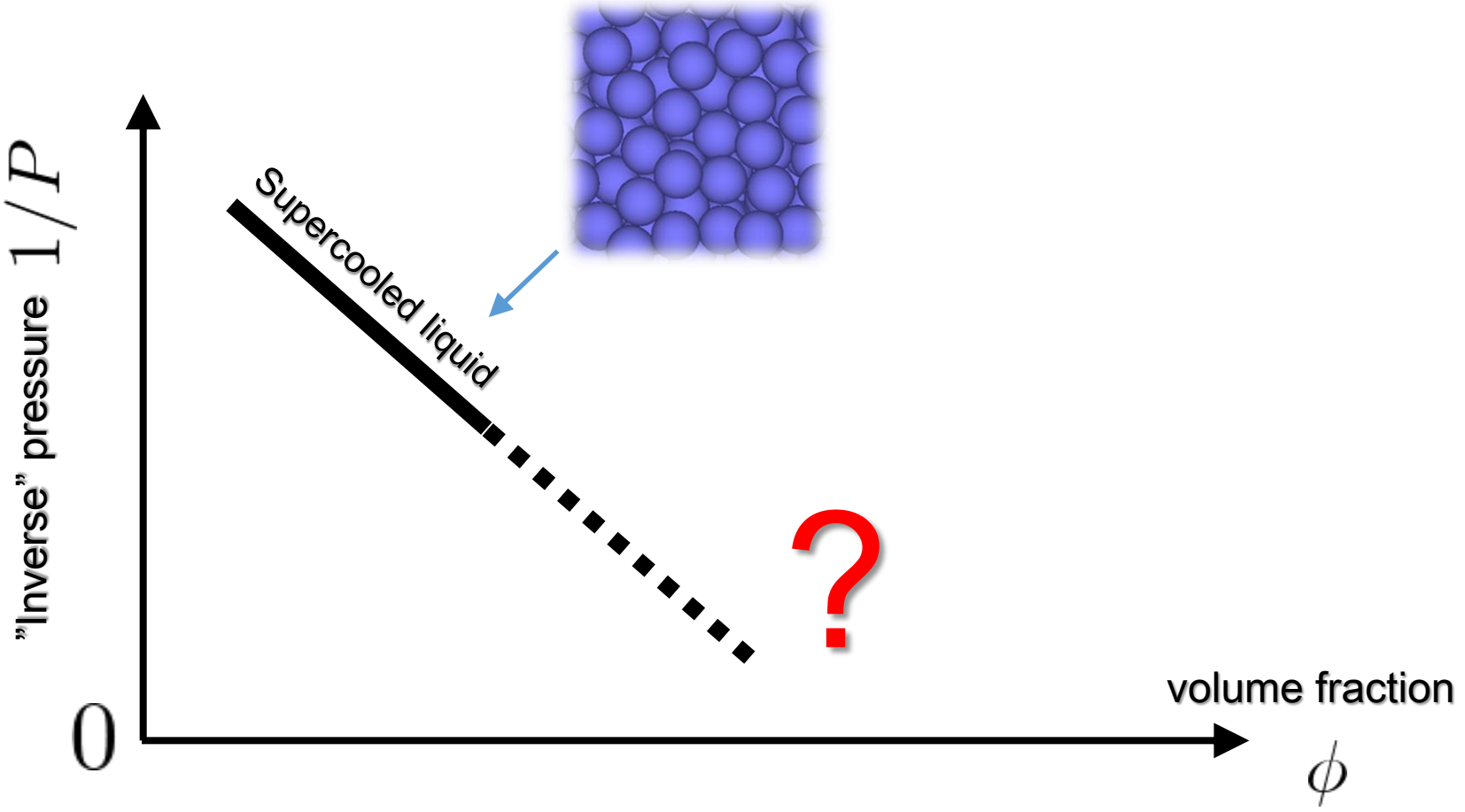


Berthier, Coslovich, Ninarello, and Ozawa, arXiv:1511.06182

Introduction: Equation of state of hard spheres



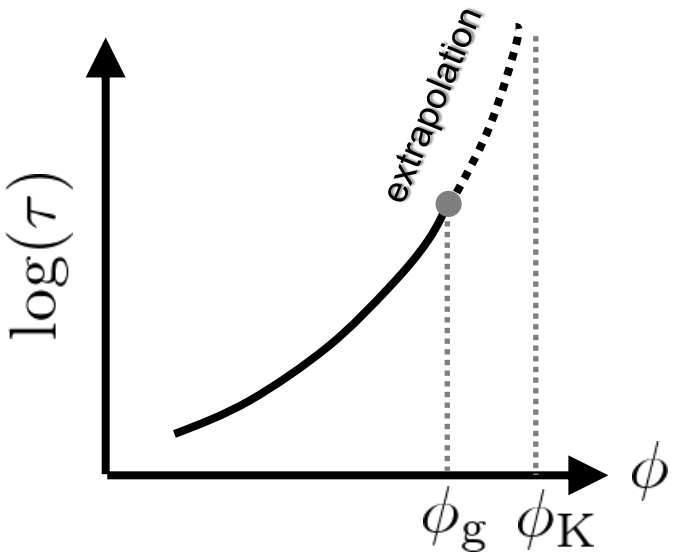
Introduction: Equation of state of hard spheres



- What is the ultimate fate of the supercooled liquid state?

Introduction: Glass and Jamming transitions

Glass transition



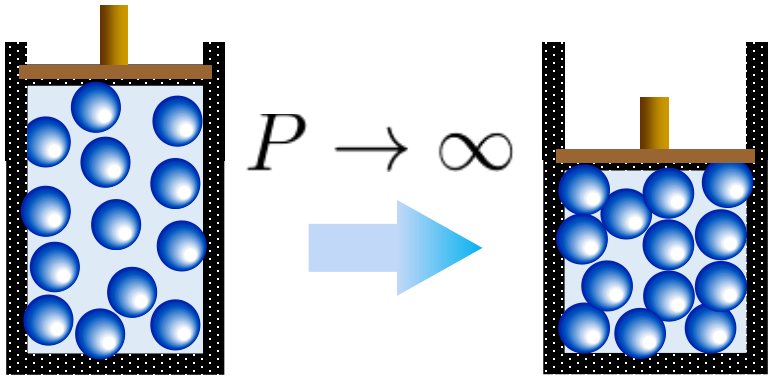
- Kinetic glass transition

$$\tau(\phi_{\mathrm{g}}) = 10^2 \text{ sec.}$$

- Ideal glass transition

$$\tau(\phi_{\mathrm{K}}) = \infty$$

Jamming transition



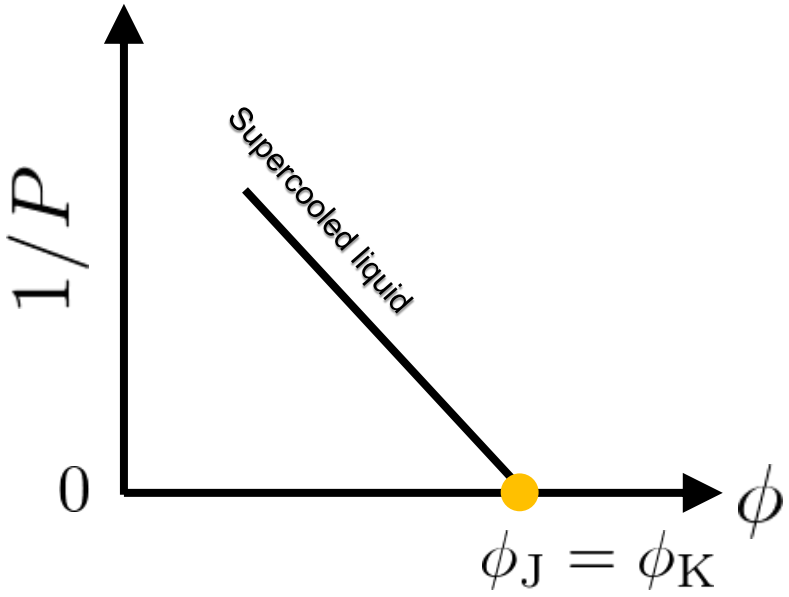
- Jamming transition density

$$\phi_{\mathrm{J}} \sim 0.64$$

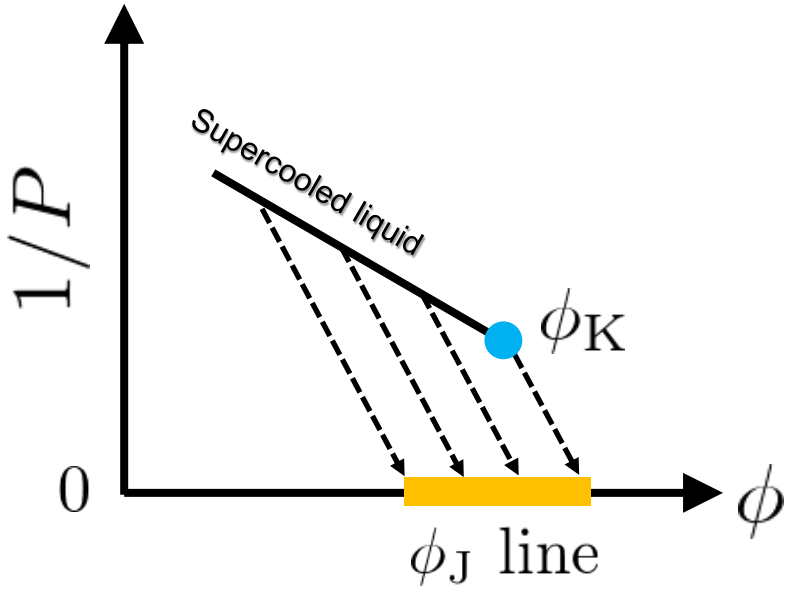
- Average contact number

$$\overline{z} = 2d \quad \text{(Isostaticity)}$$

Introduction: Two scenarios



VS



Kamien and Liu, PRL 2007

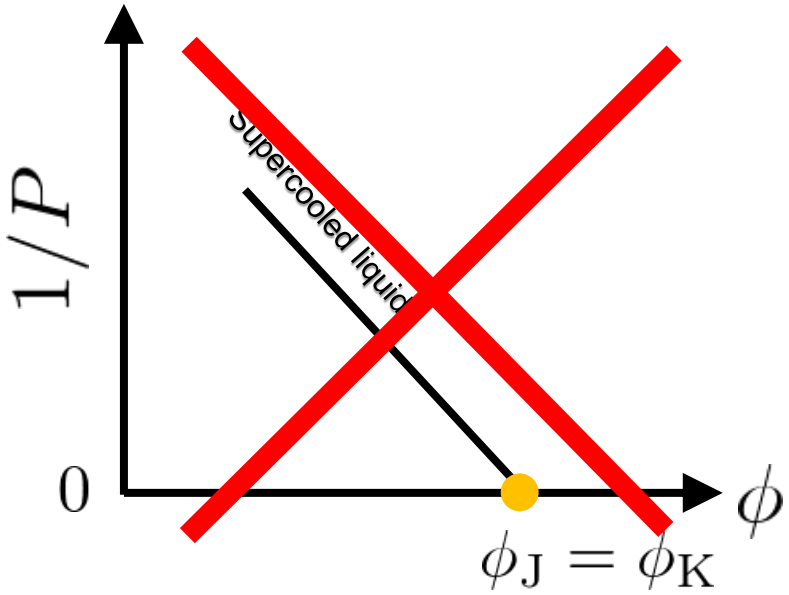
Aste and Coniglio, EPL 2004

Mari, Krzakala, and Kurchan, PRL 2009

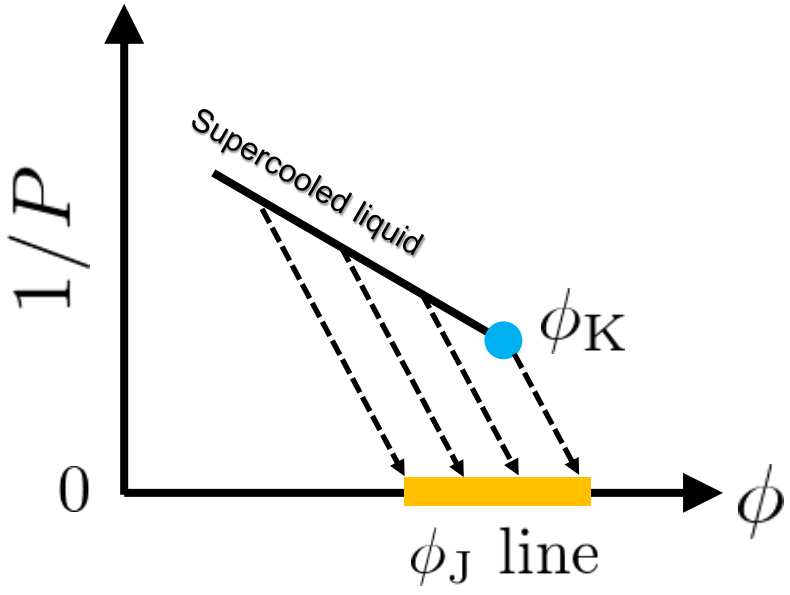
Parisi and Zamponi, RMP 2010

Motivation of this work

Making equilibrium states $\phi > \phi_J$!



VS



Kamien and Liu, PRL 2007

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Model and simulation method

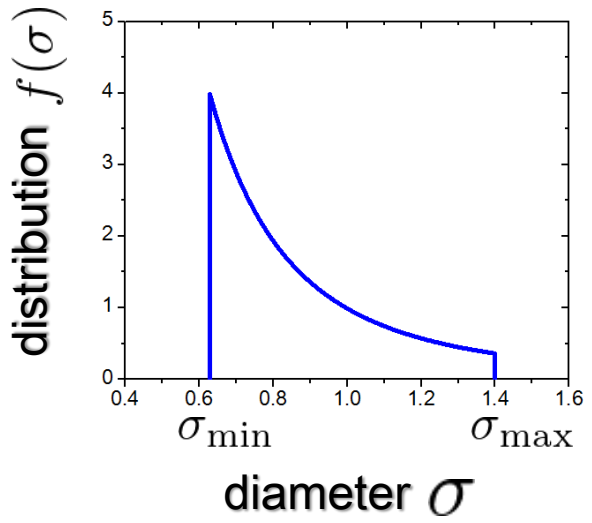
- Continuous polydisperse hard spheres

$d = 3$ with periodic boundary condition

$$f(\sigma) \propto \sigma^{-3}$$

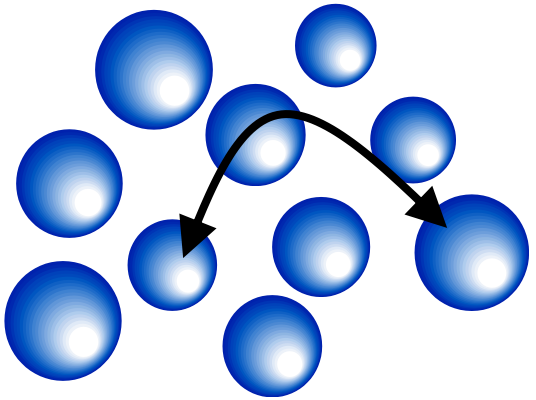
$$\delta = \frac{\sqrt{\overline{\sigma^2} - \overline{\sigma}^2}}{\overline{\sigma}} = 0.23$$

$$N = 300, 1000, 8000$$



- Equilibration algorithm

Standard Monte Carlo
+ non-local swap displacement



Grigera and Parisi, PRE 2001

Brumer and Reichman, JPCB 2004

Fernandez, Martin-Mayer, and Verrocchio, PRL 2007

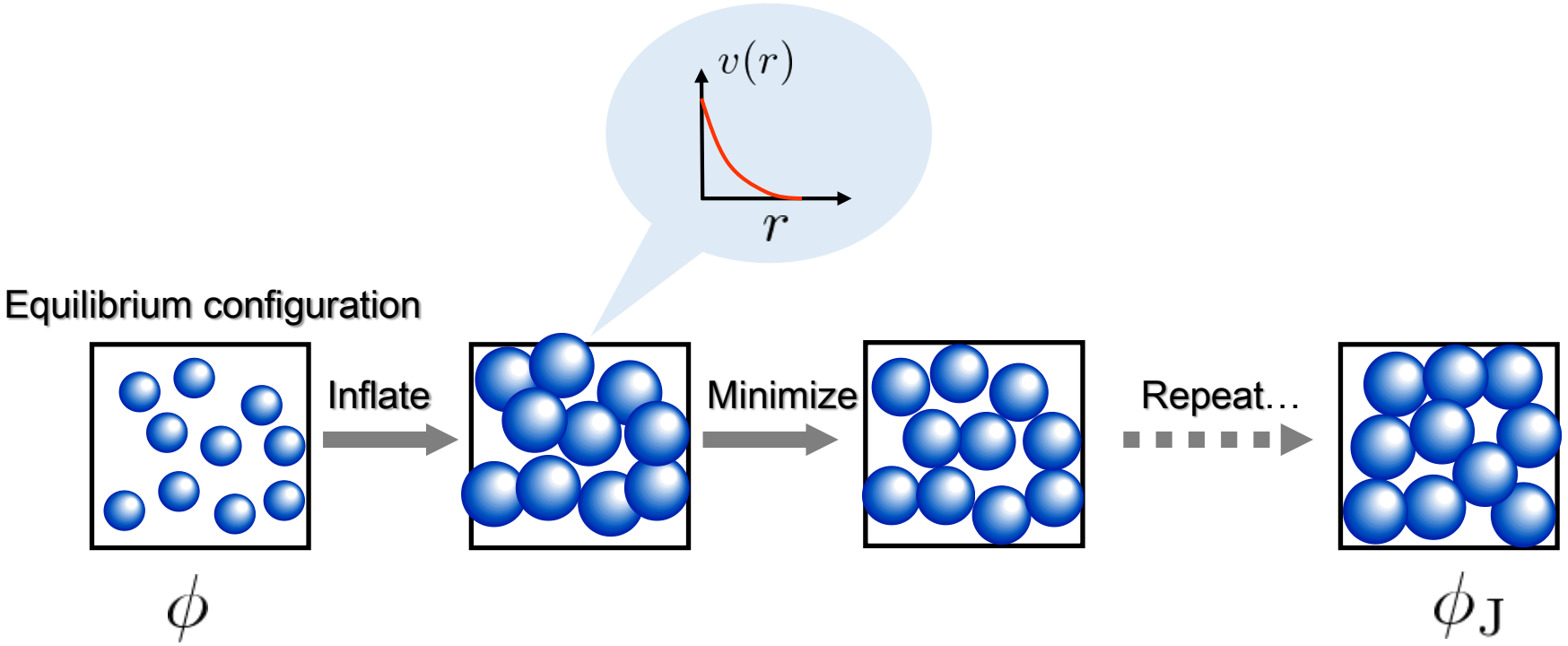
Model and simulation method

- Non-equilibrium compression algorithm for ϕ_J

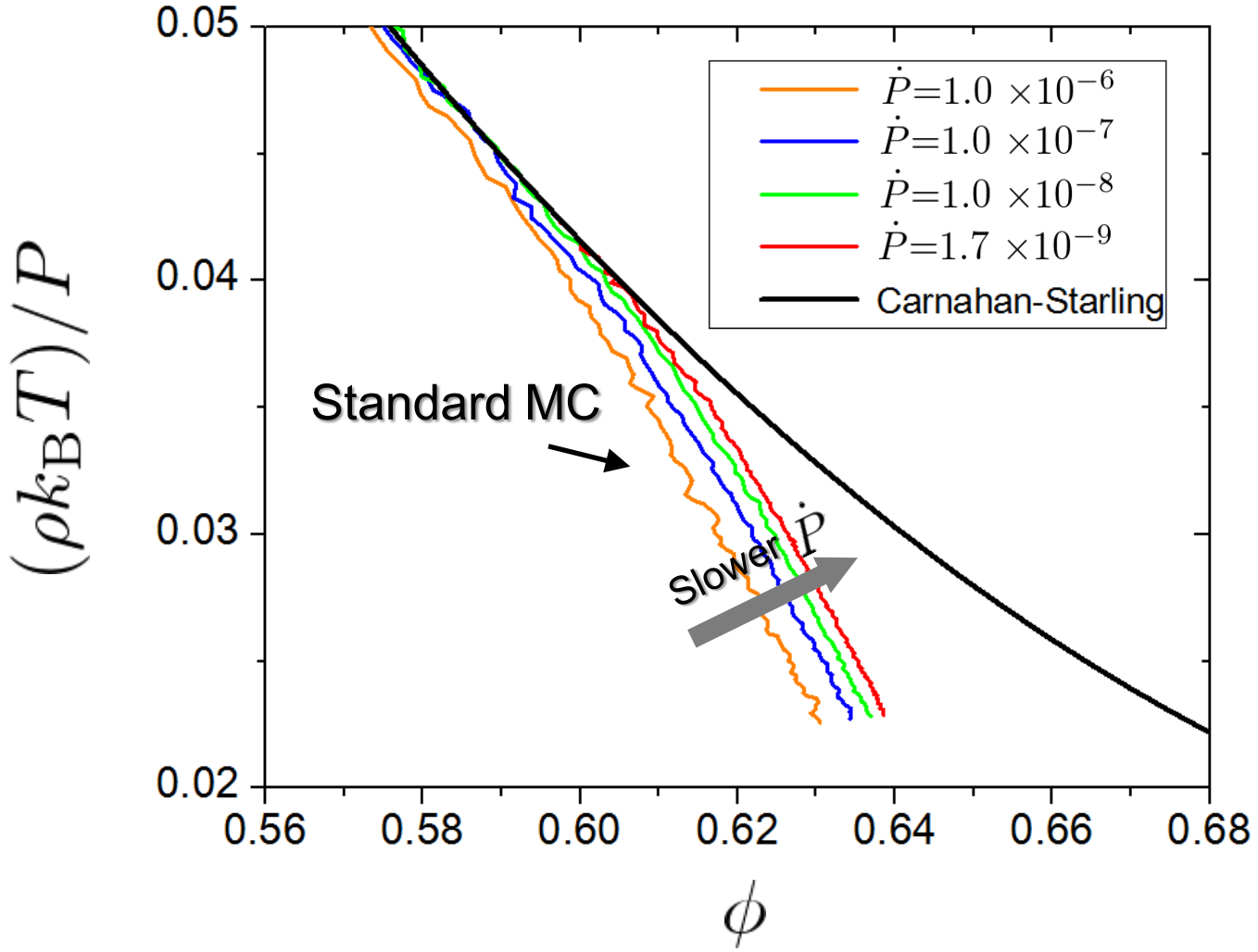
O'Hern et al., PRE 2003

Xu, Blawzdziewicz, and O'Hern, PRE 2005

Chaudhuri, Berhier, and Sastry, PRL 2010

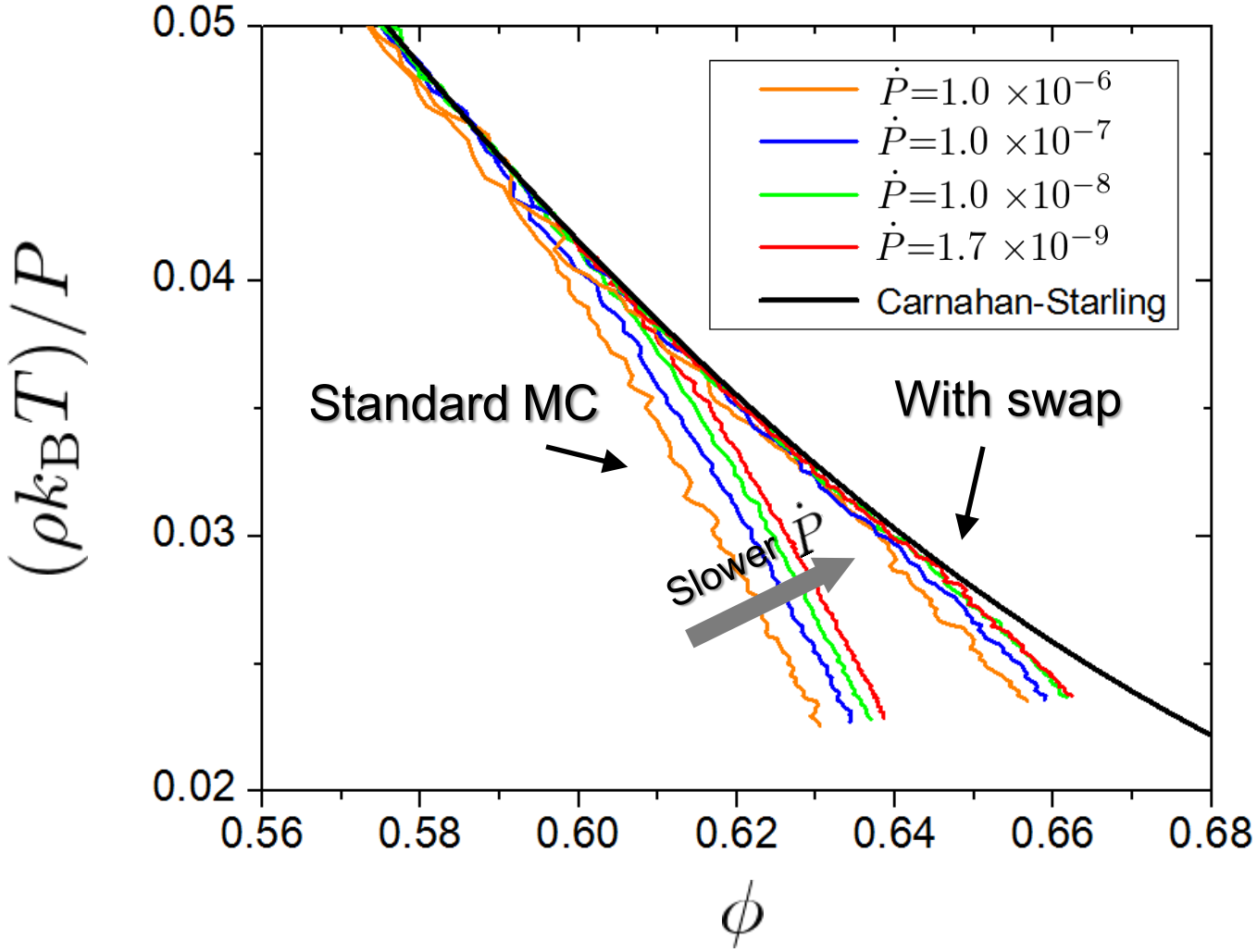


Results: Performance of the swap displacement



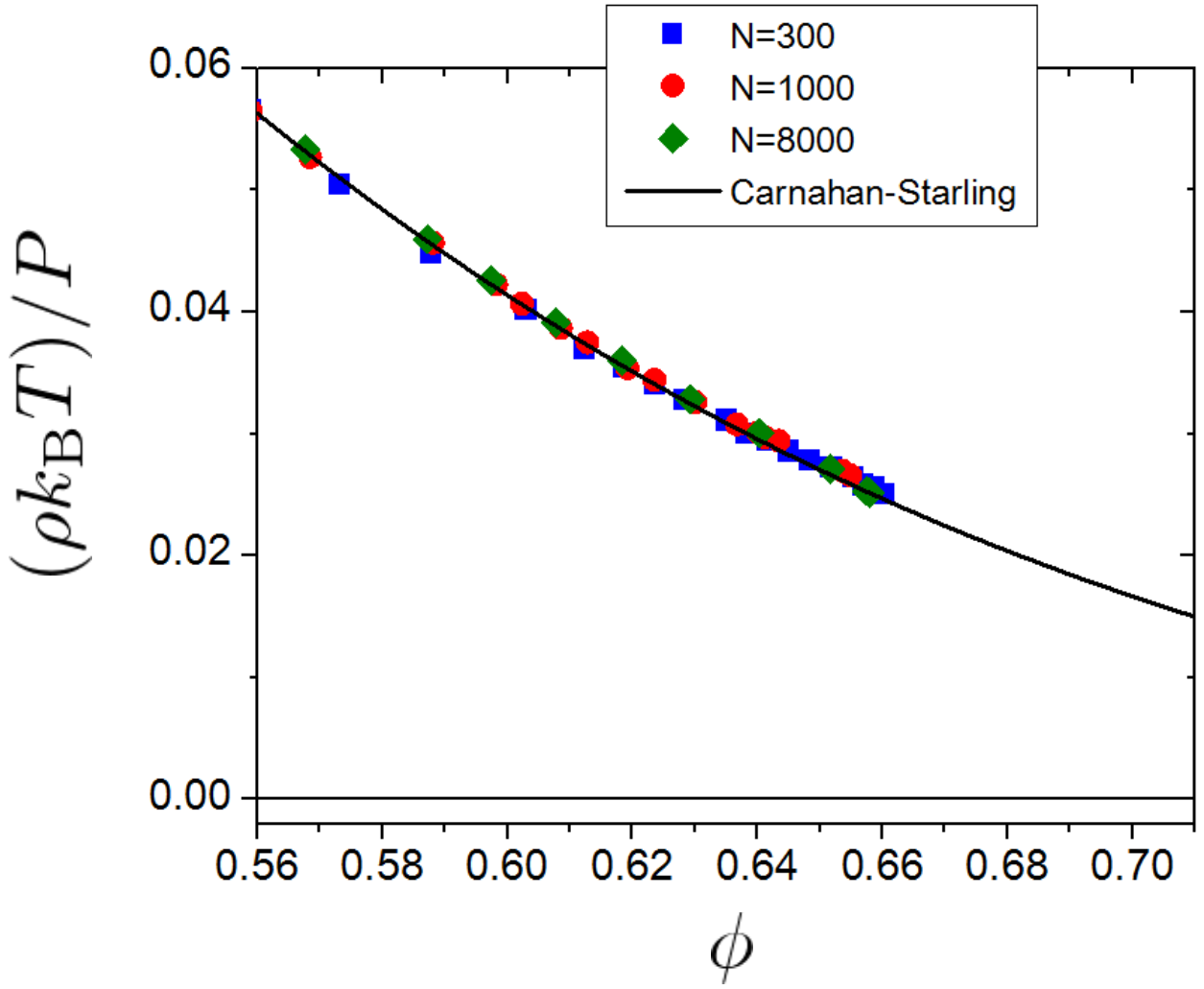
- Standard MC falls out-of-equilibrium quickly

Results: Performance of the swap displacement



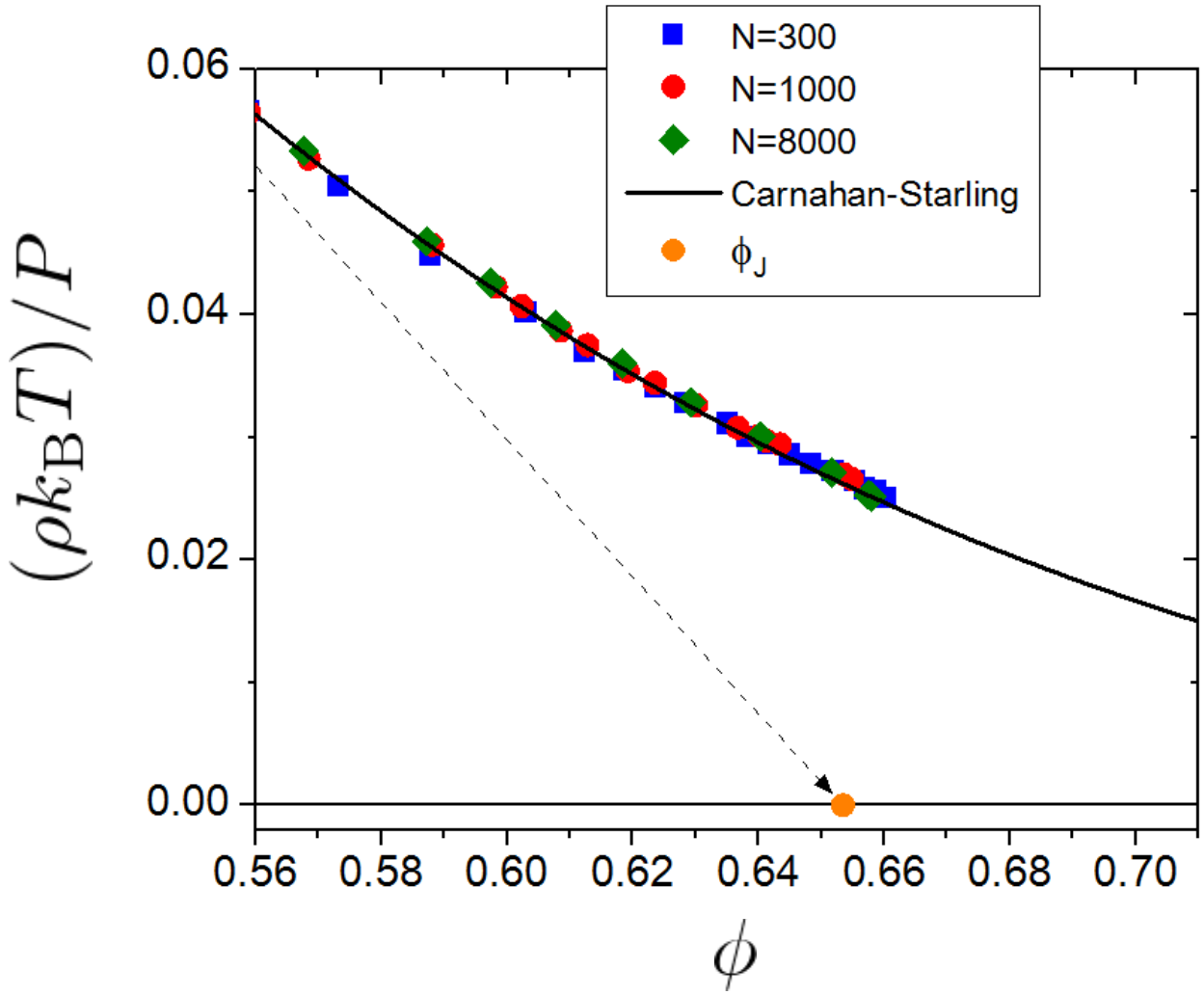
- Non-local swap displacement accelerates equilibration!

Results: Equation of state



- The system is equilibrated up to $\phi \sim 0.66$

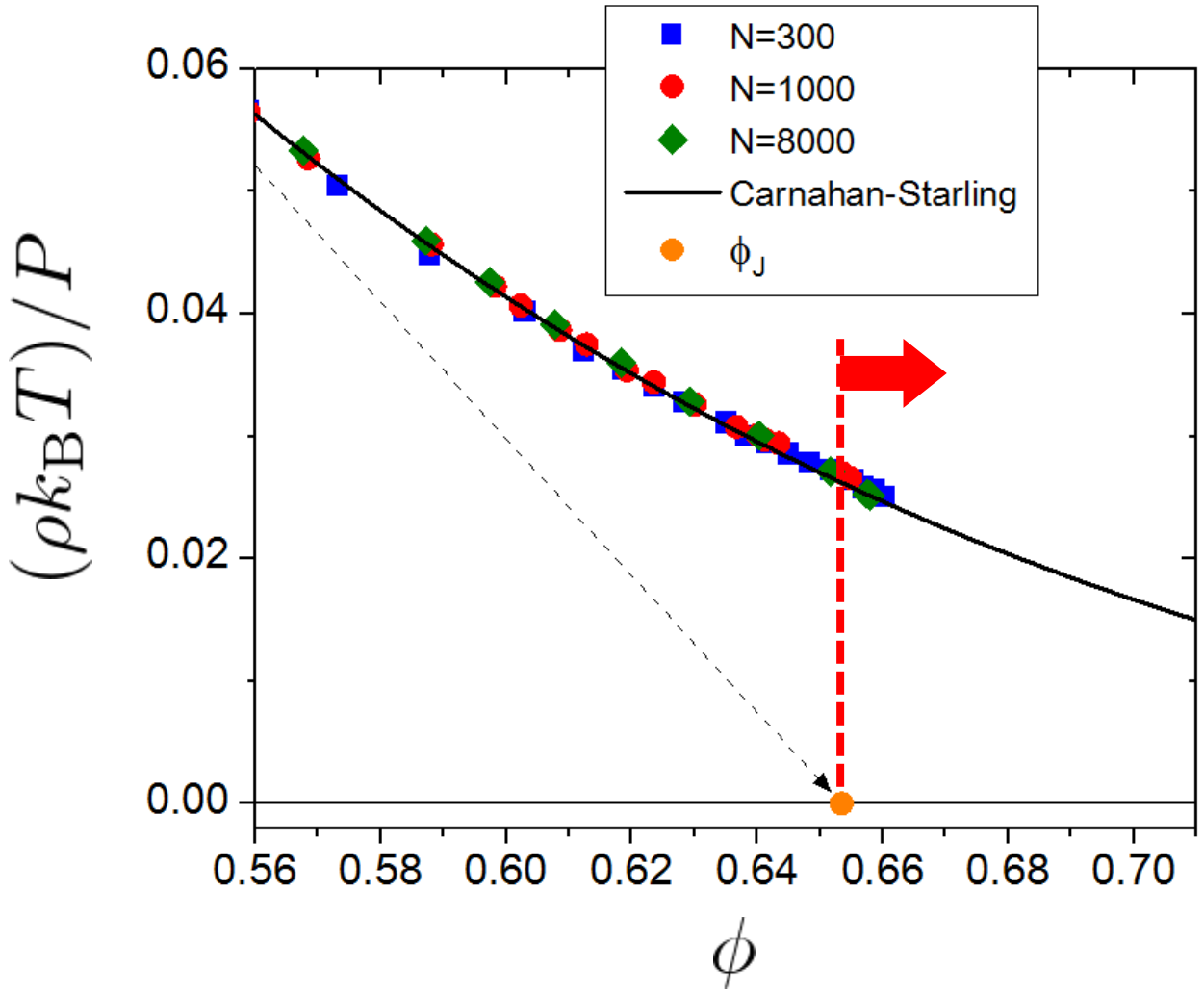
Results: Equation of state



- $\phi_J \sim 0.655$ is obtained by compressing dilute liquids

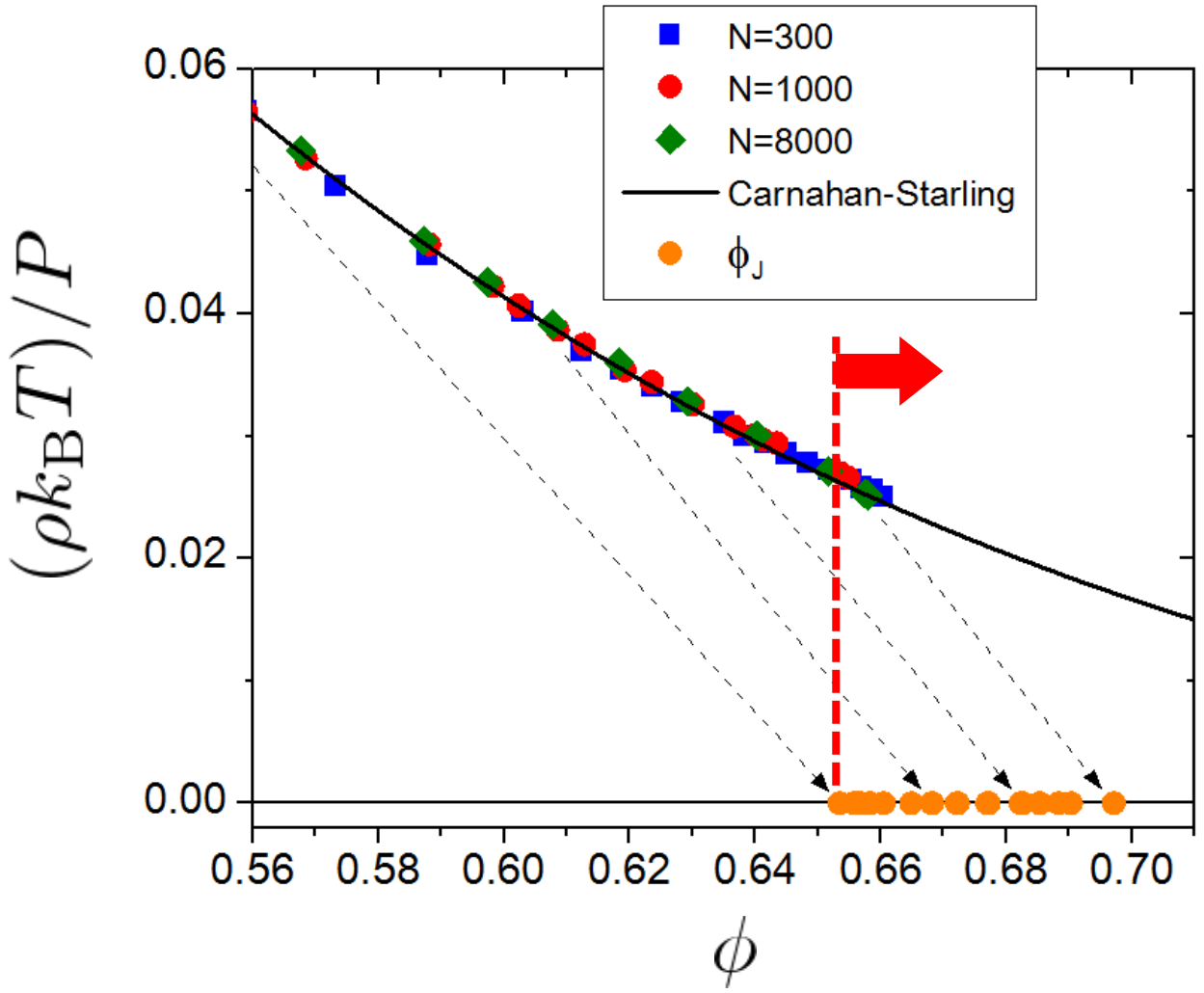
Desmond and Weeks, PRE 2014

Results: Equation of state



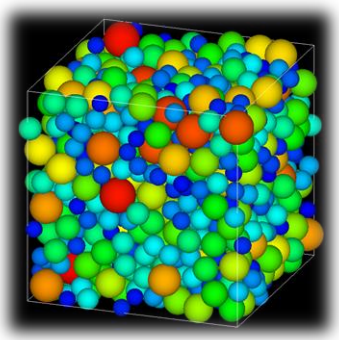
- The system is equilibrated beyond ϕ_J

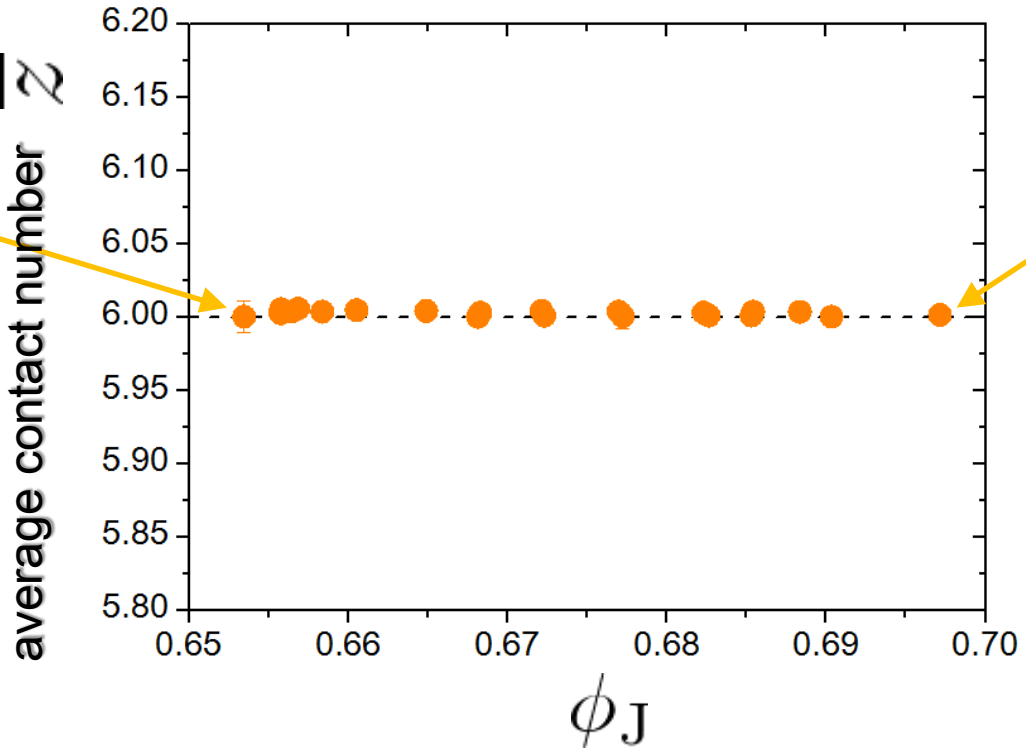
Results: Equation of state

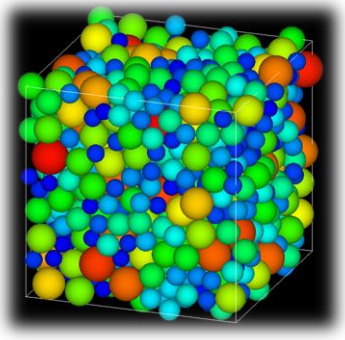


- A continuous range of ϕ_J line is obtained

Results: ϕ_J - line





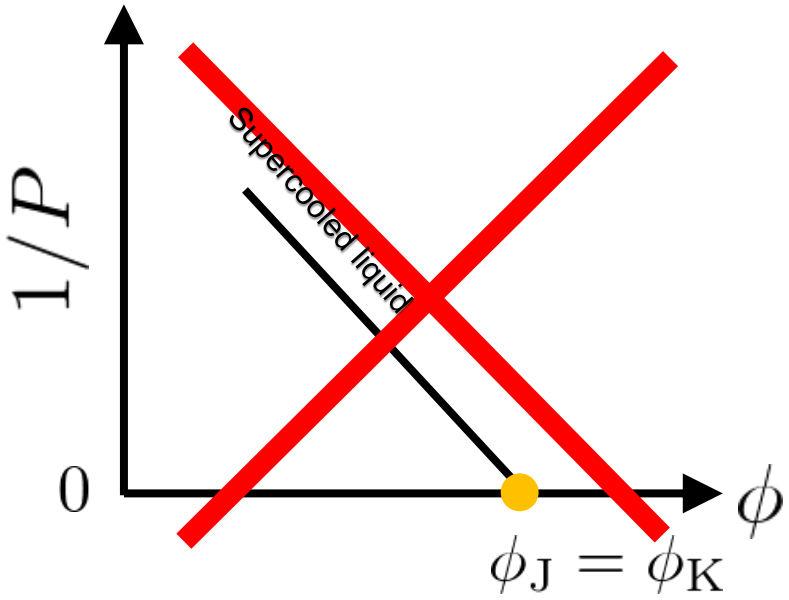


- $\overline{z} = 2d$ holds at ϕ_J - line

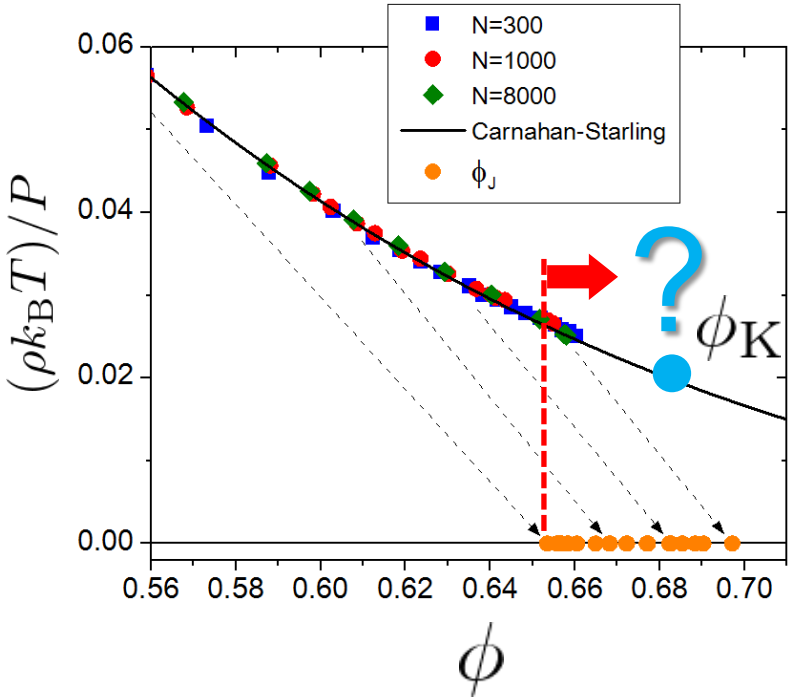
Chaudhuri, Berhier, and Sastry, PRL 2010

Ozawa, Kuroiwa, Ikeda, and Miyazaki, PRL 2012

Conclusions



VS



- Related work:
  Glass-to-jamming transition

- Future work:
  Does the ideal glass transition density ϕ_K exist?